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Machine Learning and Supercomputing to Predict Corrosion/Oxidation of High-Performance Valve Alloys

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Project ID# 162

ORNL is managed by UT-Battelle, LLC
for the US Department of Energy

Overview

Timeline

- Project start: Oct 2018
- Project end: Sep 2021
- Percent complete: 15%

Budget

- Total project funding: $1,935K
  - DOE share: $1,500K
  - Cost share: $ 435K
- Awarded for 3 years (FY19-FY21)
- FY 2019: $500K

Barriers

- Absence of physics-based model to predict high-temperature alloy oxidation
- Lack of fundamental alloy oxidation data (e.g., atomic mobilities in oxides, oxygen permeability)

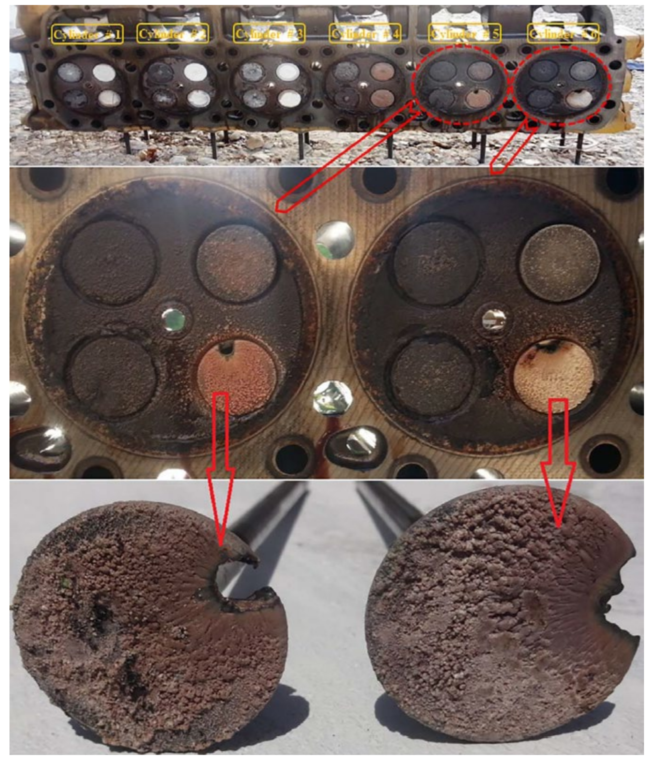
Partners

- ASM International
- Penn State University
- Federal-Mogul Powertrain

Any proposed future work is subject to change based on funding levels.

Increased exhaust temperature for engine efficiency will require advanced corrosion/oxidation-resistant alloys

Oxidation damage in IN751 valves at ~850°C*



*estimated

M.I. Khan et al. Engineering Failure Analysis 85 (2018) 77–88

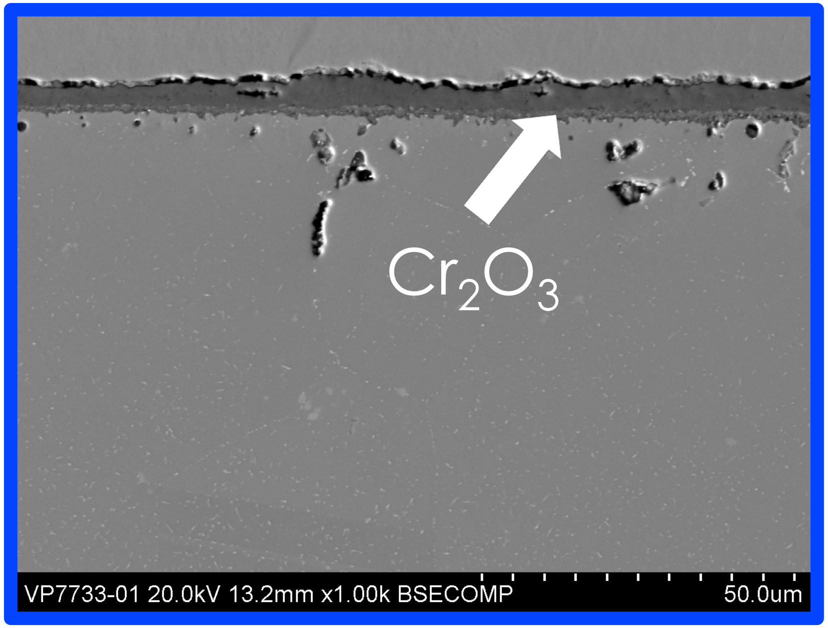
Natural gas engine operated for 10,000 h

Strategy to mitigate high-temperature oxidation?

Thermally grown thin and coherent oxide scales to protect alloys from extreme environments

Sanicro25

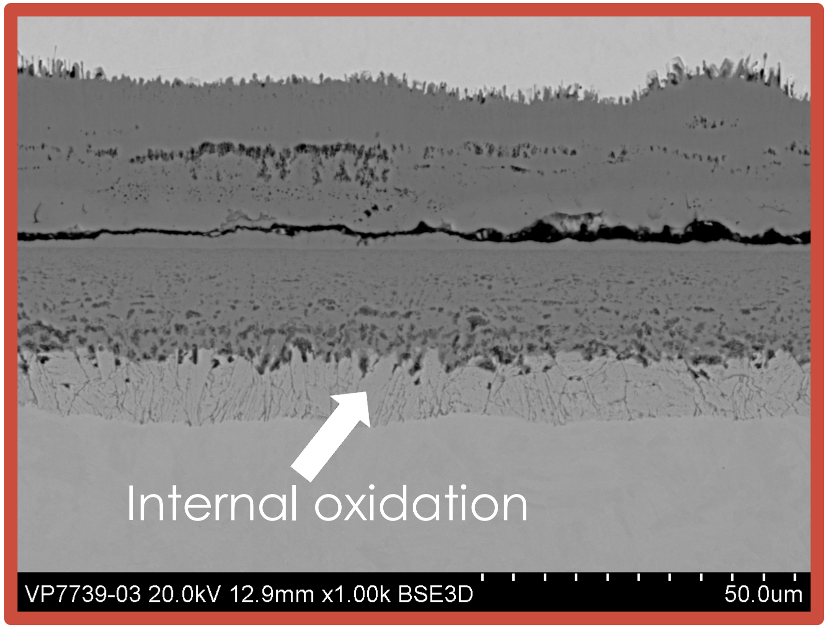
22Cr25NiWCoCu stainless steel



Good

Gr91

9Cr1Mo steel



Bad

Is it possible to predict high-temperature alloy oxidation?

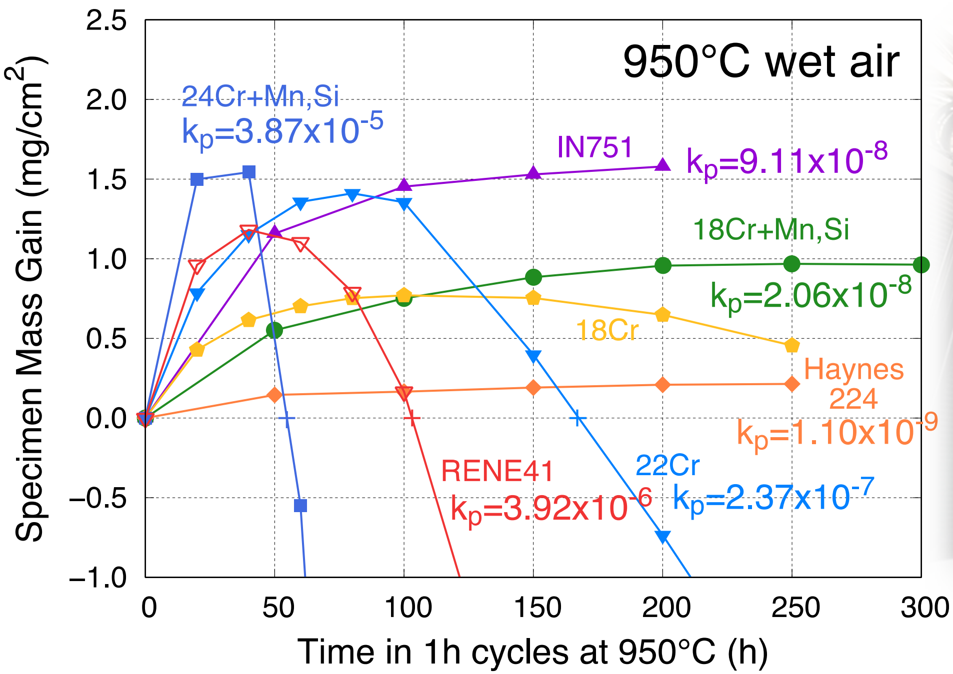
First-principles bottom-up design of oxidation-resistant multi-component alloy is not yet possible

Alloy thermodynamics	Alloy diffusion kinetics	Oxide thermodynamics
• alloy phase diagrams	• precipitate coarsening	• oxide phase diagrams

Oxide diffusion kinetics	Alloy thermodynamics with oxygen
• metal cation mobilities • grain boundary diffusion	• oxygen permeability • oxygen mobilities

Predictive models for alloy oxidation are not available due to the lack of fundamental experimental data

Leveraging ORNL's high-quality experimental oxidation data with modern supercomputing



This project aims to develop predictive models as accurate as cyclic oxidation experiments relevant to automotive applications

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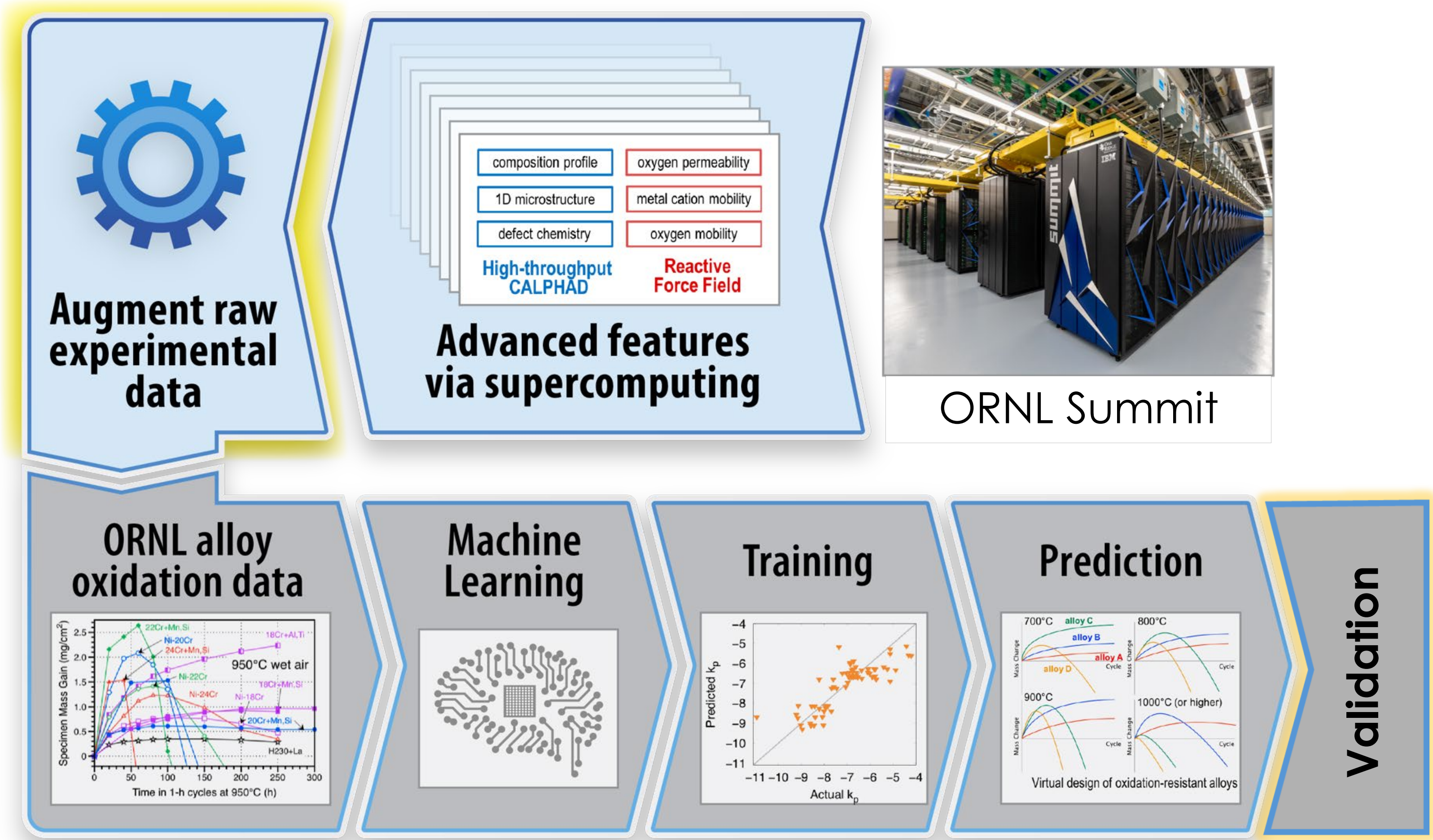
ORNL's 20yrs+ high-quality experimental data coupled with advanced scientific alloy features



Proposed workflow is anticipated to go beyond Ni-Cr alloys (e.g., stainless steel and Ni-Al alloys)

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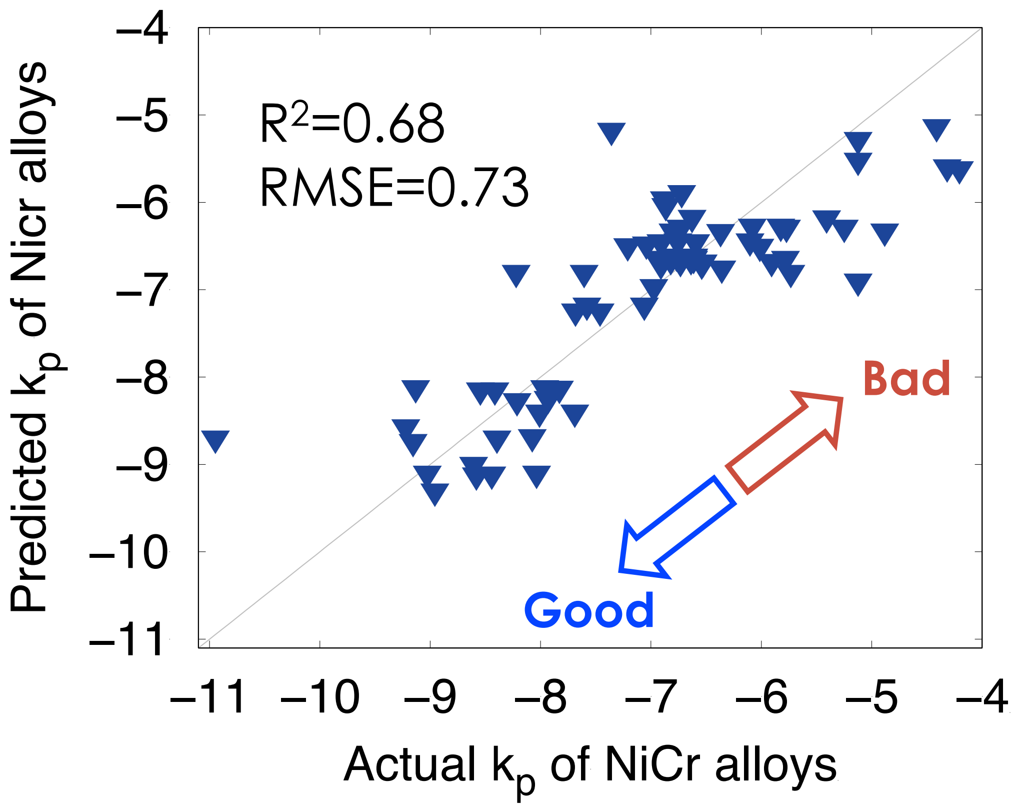
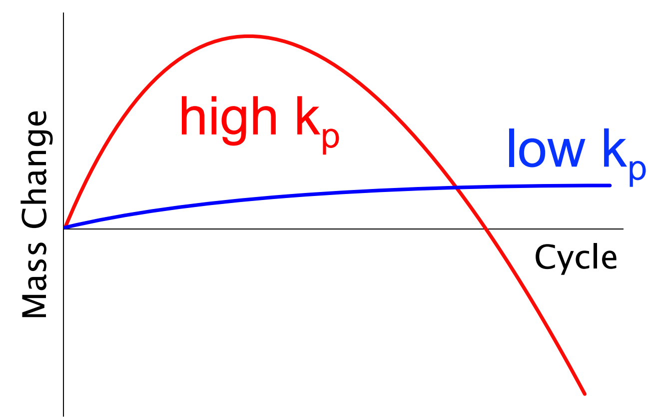
Successful training of preliminary machine learning models to predict rate constant (k_p)

<u>78 Ni-Cr alloys at 950°C (10% H_2O)</u>



- <u>input:</u> alloy chemistry (Ni, Cr, Co, Mo, Mn, Fe, …)
- <u>output:</u> alloy oxidation rate constant (k_p)



Predictive, but features other than compositions are needed to better understand fundamental alloy oxidation mechanisms

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Collaboration and Coordination

World-class research teams to develop alloy oxidation model with 20+ years data and supercomputer

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Computational Thermodynamics/ Diffusion Kinetics

Data Analytics and Supercomputing

ASM International

Data Repository

PennState

Atomistic Simulations

Federal-Mogul Powertrain

Finite Element Analysis

Monthly all-hands conference call, biweekly subtask team meetings

Project will focus on generating alloy features to be correlated with ORNL's high-quality experimental data

High-throughput CALPHAD

- Populate **scientific alloy features**
  - Depletion of major elements (e.g., Cr)
  - Dissolution of key strengthening precipitates
  - Temperature excursion

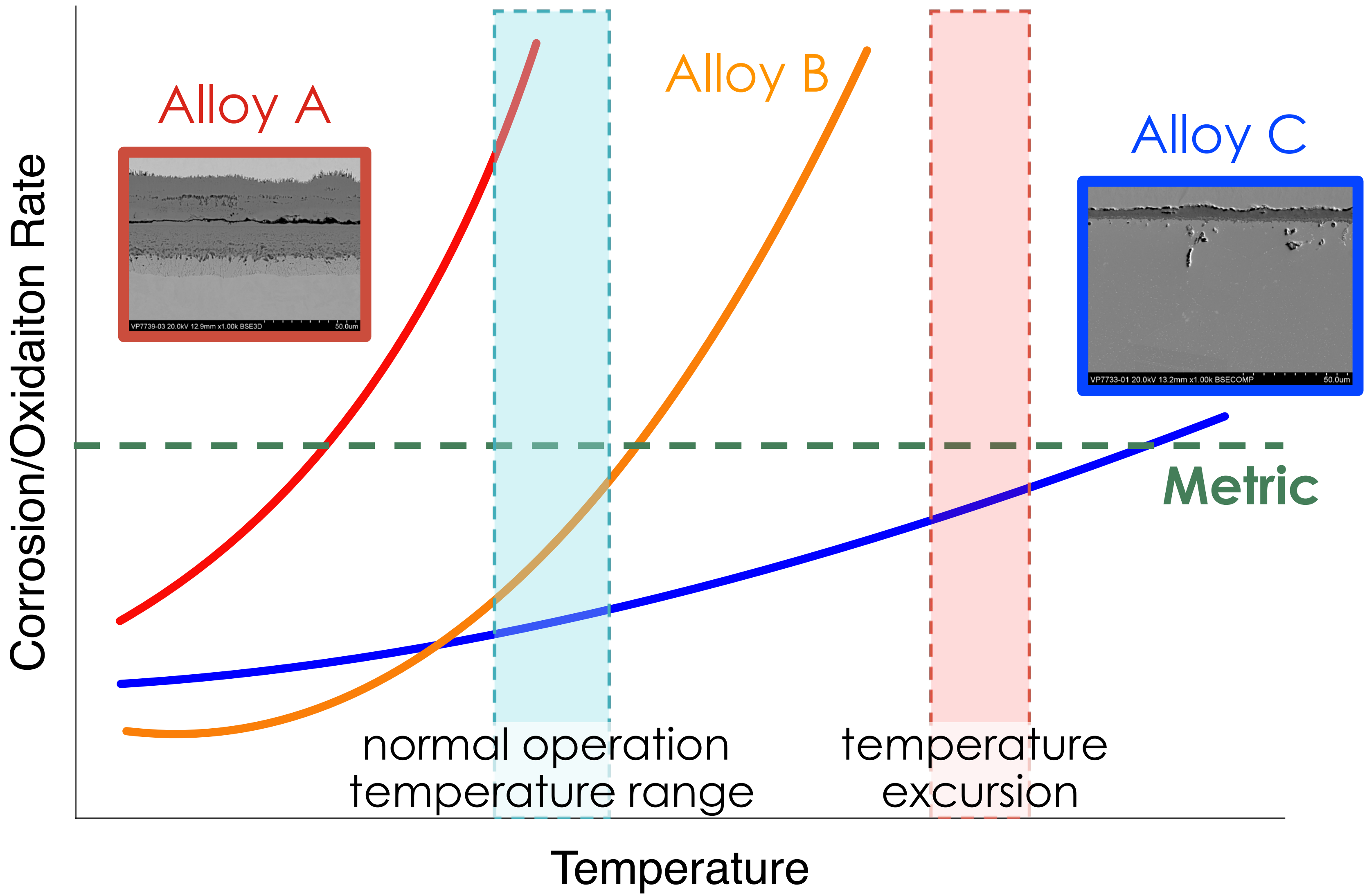
High-fidelity Atomistic Simulations

- Generate **fundamental oxidation data** via Reactive Force Field (ReaxFF) simulations
  - Oxygen permeability
  - Grain boundary diffusion

Data analytics

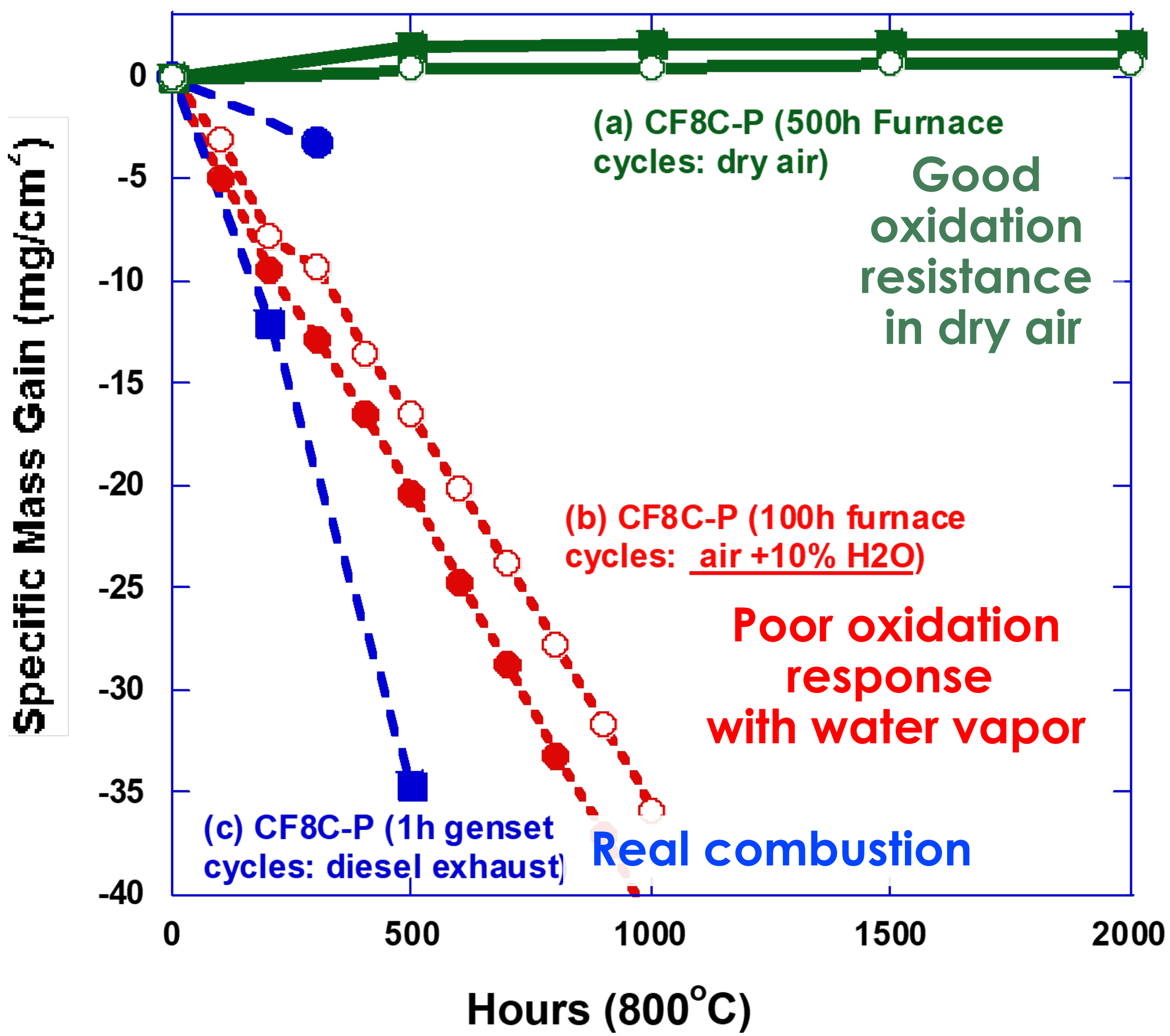
- Analyze correlation between input features and alloy oxidation
- Train machine learning models with identified **key features**

Develop practical alloy oxidation model with 20yrs+ ORNL data, machine learning and supercomputing



Technical Backup

Laboratory simulated 10% water vapor testing can mimic real combustion environment



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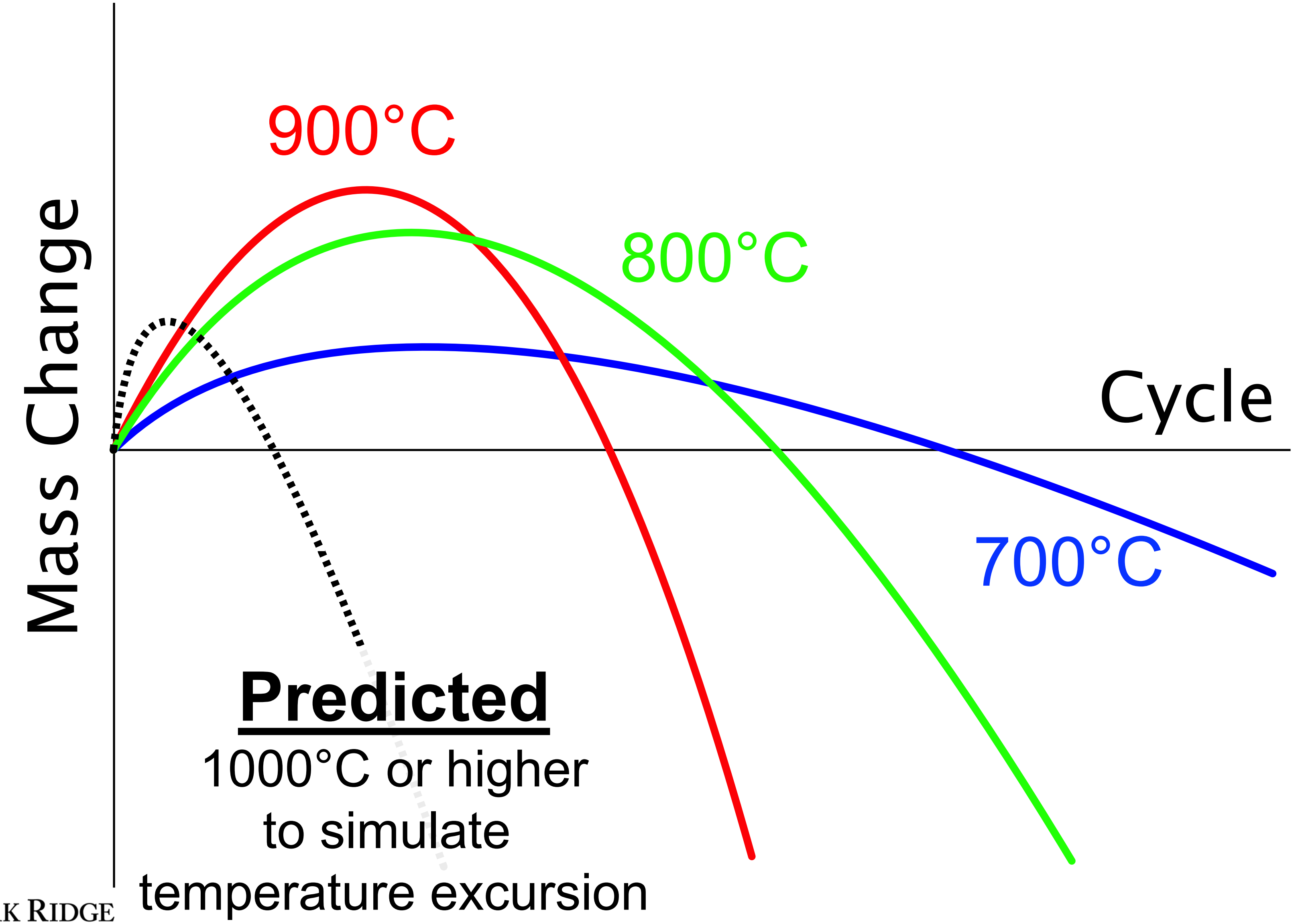
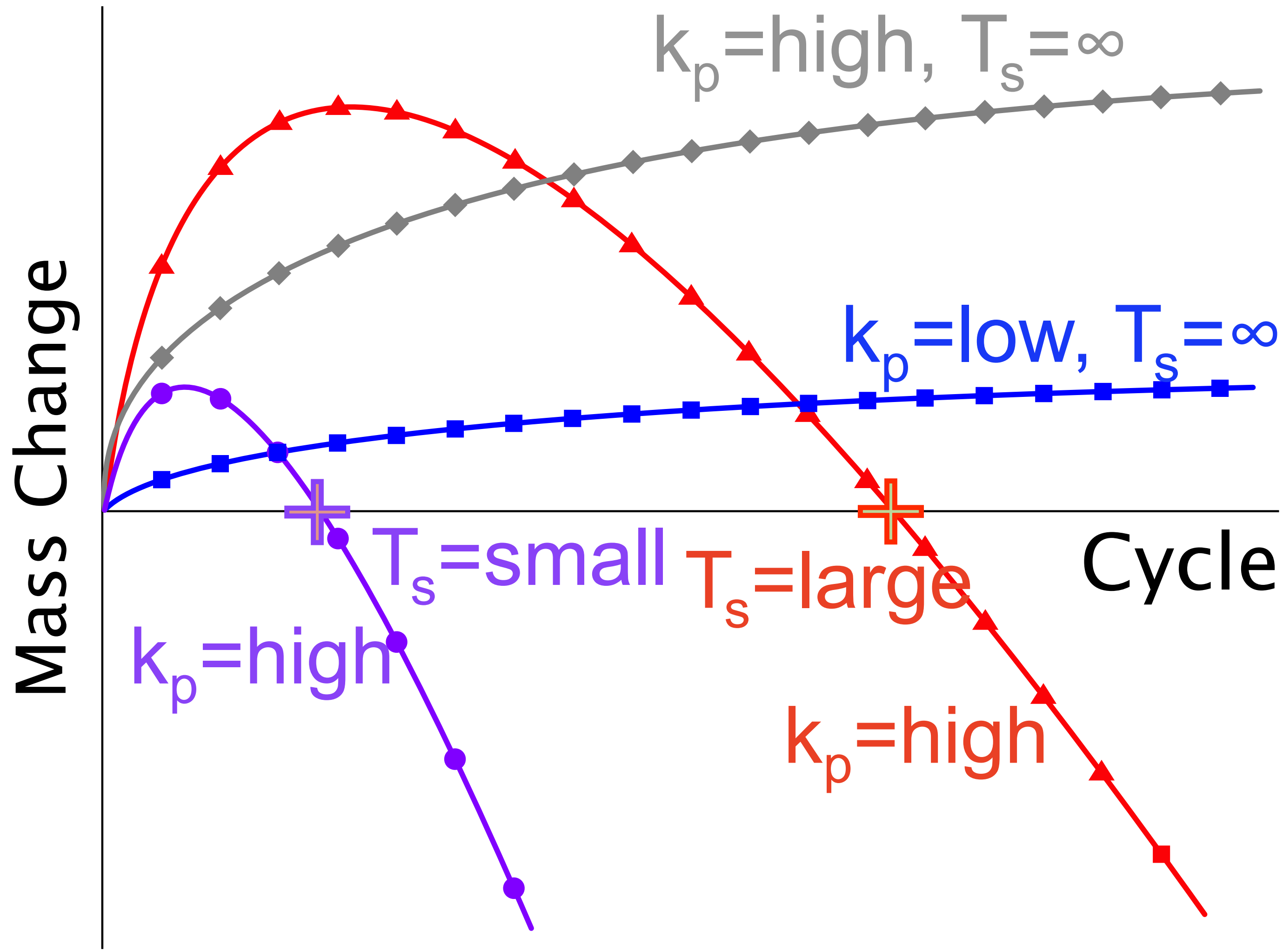
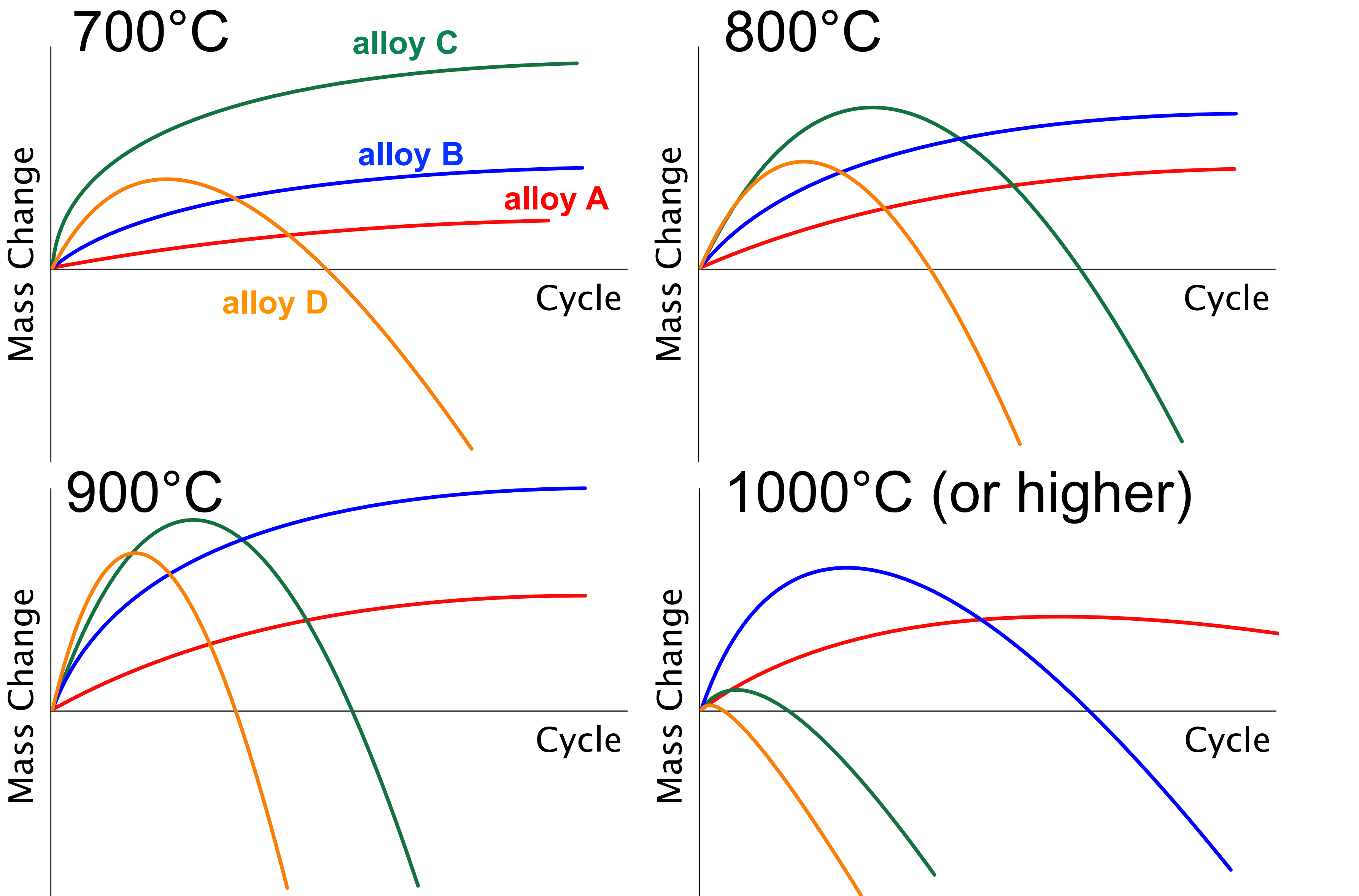
Temperature effect on oxidation behavior of high-temperature alloys



We propose using k_p (rate constant) and T_s(time/cycle to spall) to represent oxidation behavior of alloys



Alloy chemistry and temperature dependent k_p and T_s prediction



Catalog of ORNL's experimental data for 10% H_2O cyclic oxidation NiCr alloys: total 337 data

Temp (°C)	Model alloys	Commercial alloy data*	
800	32		
850	23	15	N80, N90, 31V & 751 (2~4) R41 & WASPalloy (1)
900	40	45	247 (21), 751, 214, 31V, R41, 282, N80 & WASPalloy (2~4), U520, U720, 230, N90 (1)
950	18	64	751 (11), N80 (9), U520 (6), 247 (5), R41 (5), 214, N90, 246, 713, 282 & U720 (2~4) 230 & WASPalloy (1)
1000		8	246, 247 & 713 (2~3), N90 (1)
1050	4		
1100	16	42	247 (42)
1150	15	12	247, 214, 224 & 230 (2~4), 713 (1)
1200		6	247 (6)

*() – individual data count

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